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RPPR Final Report
as of 22-Aug-2018

Agency Code:

Proposal Number: 67891EV **Agreement Number: W911NF-15-1-0598**

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Report Date: 14-Dec-2016 Date Received: 05-Jul-2018
Final Report for Period Beginning 15-Sep-2015 and Ending 14-Sep-2016
Title: Toward Accurate Models of Wet Granular Media in Nature
Begin Performance Period: 15-Sep-2015 **End Performance Period:** 14-Sep-2016
Report Term: 0-Other

Submitted By: Kenneth Kamrin Email: kkamrin@mit.edu
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Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: **STEM Participants:**

Major Goals: This short project was aimed at discrete and continuum simulation methods for wet granular materials. The project explored modeling of slightly wet grains (i.e. the pendular regime) and fully saturated grains. These two areas were treated as two separate problems.

On the partially wet side, the first goal was to write a novel and robust discrete element method that captures fluid bridging, fluid transfer during contact breaking, and time-dependence of bridge formation, simultaneous with frictional contact modeling of grain-on-grain interaction. Once achieved, the discrete method can be used like an experiment to identify homogenized continuum relations.

On the fully saturated side, our aim was to develop an effective LBM-DEM method that could be used to provide inputs to a poro-plastic type continuum model. The goal was to cast the continuum model within a meshless numerical framework that permits huge deformations. Transitioning a finite-element poro-plastic approach to a meshless one would utilize the consultation of Prof David Henann at Brown, a finite-element expert. Geoscientist Dr. Colin Stark at NYU would help with the selection of natural particle-scale input parameters.

Accomplishments: Many of the goals proposed were accomplished, though some of them materialized after the close date of the short grant.

On the discrete side, were able to write and implement a custom method that tracks the fluid layer thickness on each grain as a separate degree of freedom. During contact, the layer thicknesses of the contact pairs evolve dynamically as fluid is (viscously) driven into the bridge. As the bridge is forming, the strength of the bridge itself is evolving with it as a function of bridge volume. The current bridge volume is appended to the discrete system as a new "contact" variable. This approach not only captures the effect of fluid viscosity on bridge dynamics, but also guarantees fluid mass conservation and realistic fluid redistribution onto grains when bridges break. Using this method we were able to identify a rheological form based on two dimensionless numbers: The inertial number I_1 and the wetness number I_2. The number I_1 is standard from dry granular flow, and it measures the competition between the time-scale of the macroscopic strain-rate and the pressure-driven rearrangement time. The number I_2 invokes the fluid surface tension and compares it against the system pressure. We were able to identify the normalized flow resistances in terms of these two numbers to provide a closed rheology.

As for the fully saturated work, we identified several nuances in the LBM-DEM framework that required close attention and specialized numerical conditioning. These helped us simulate saturated particles flowing through complex and deformable geometries. A broad continuum simulation effort was started in parallel that worked to transition existing poro-plastic FEM modeling into a meshless mixture theory. This mixture approach broadens the theory by not requiring quasi-static fluid balance, and numerically the meshless method, based on the Material Point Method (MPM), enables us to go to extreme deformations beyond the FEM limit. We have recently completed this model and numerical approach, but its genesis was during this short project period. We are now capable of simulating arbitrary grain sediment problems in the continuum, tracking both the homogenized fluid motion and the separate homogenzied grain motion.

Training Opportunities: The grant was used to co-fund two postdoc (Ramin Ghelichi and Patrick Mutabaruka) and co-fund one graduate student (Sachith Dunatunga). During this period these three personnel attended conferences and presented their work across the US.

Results Dissemination: The results were disseminated in multiple conference presentations (APS and SES). No journal articles were submitted during the one-year duration of the award, though afterward, the work done during the award duration resulted in two published/submitted papers.

Honors and Awards: Kamrin received the Eshelby Mechanics Award for Young Faculty during the award duration. This distinction is awarded jointly by ASME and the University of Houston.

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: Faculty
Participant: David Henann
Person Months Worked: 2.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Staff Scientist (doctoral level)
Participant: Colin Stark
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)
Participant: Patrick Mutabaruka
Person Months Worked: 4.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

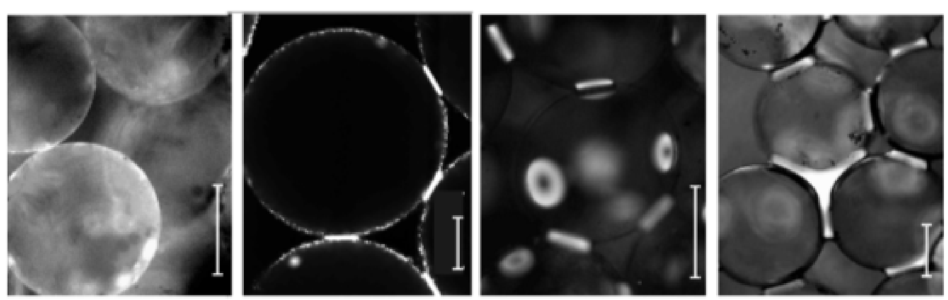
Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)
Participant: Ramin Ghelichi
Person Months Worked: 3.00 **Funding Support:**
Project Contribution:

International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Sachith Dunatunga
Person Months Worked: 3.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

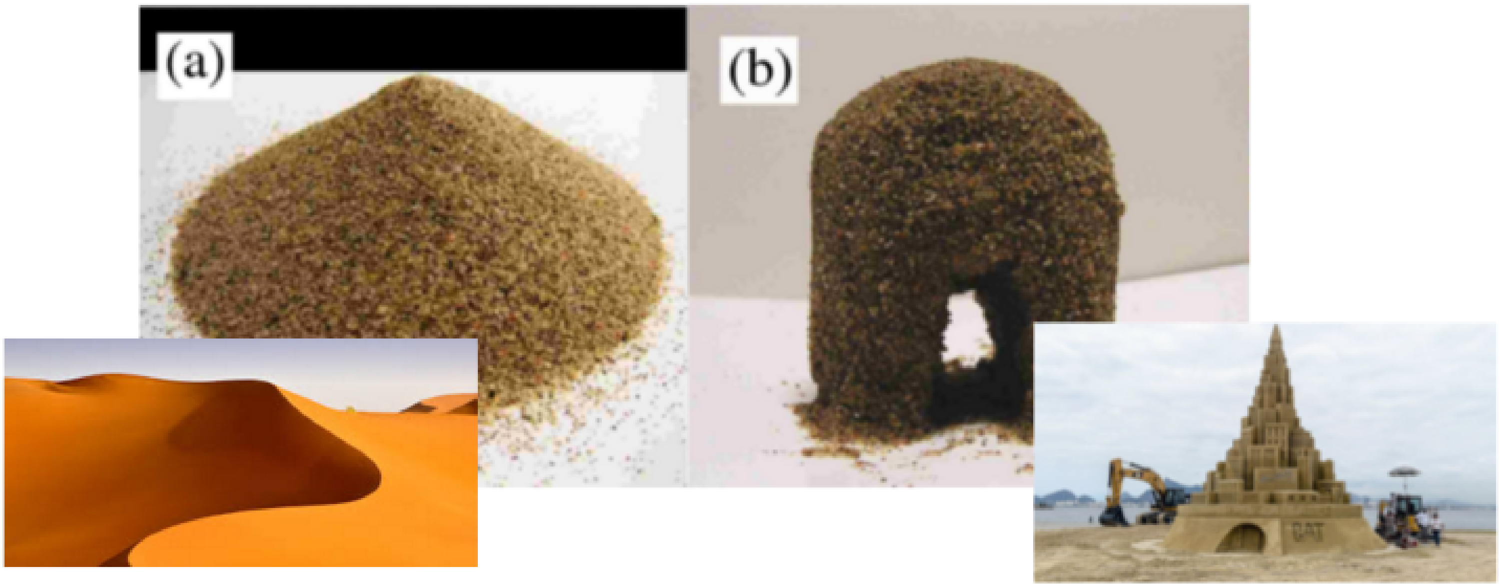
Partially-wet regimes:

wetness regime	morphology	liquid content	
humidity	asperities		$W = 0.0$ to 0.026
humidity	roughness		
		W_{cb}	
pendular			
		W^*	
funicular		clusters	0.026 to 0.08
funicular		bicontinuous	0.08 to 0.28
bubbles			0.28 to saturation



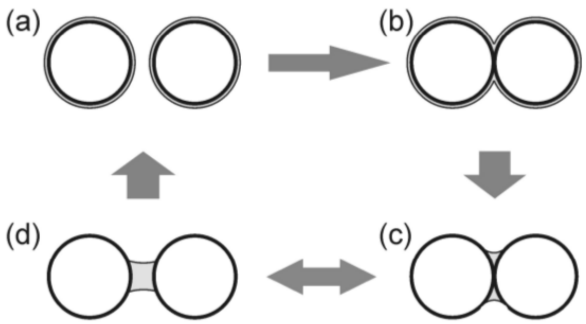
(a) (b) (c) (d)

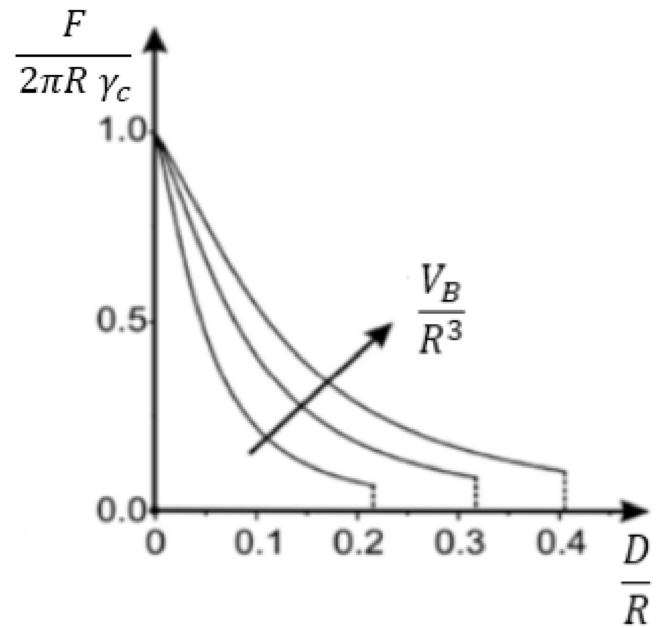
Mitirai and Nori (2007)



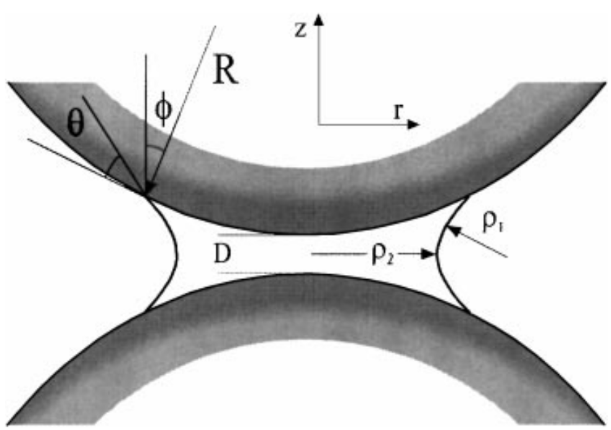
Mitirai and Nori (2007)

Capillary bridge force



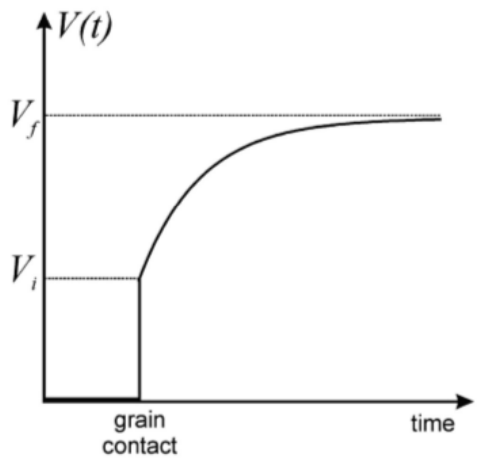


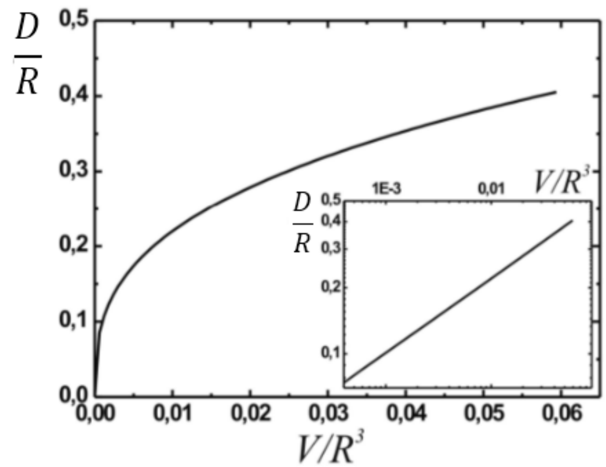
Herminghaus (2005)



$$F_{cap} \approx 2\pi R\gamma_c \left[1 - \frac{1}{\sqrt{1+\frac{2V_B}{2RD^2}}}\right]$$

Bridge Volume

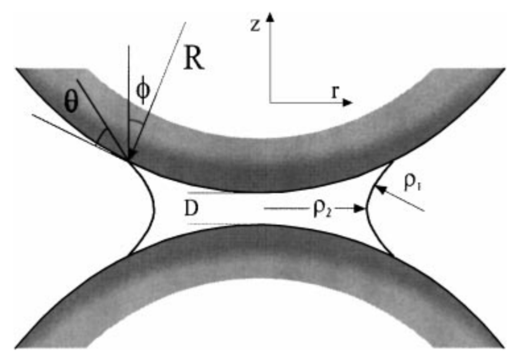




Herminghaus (2005)

$$V_B(t) = V_f\left[1 - exp\left(-\frac{C_0 h_{ij}^3}{V_f \eta} t\right)\right]$$

$$D_c \approx R(1 + \tfrac{\theta}{2}) V_B^{1/3}$$



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Customized DEM

A customized potential added to LAMMPS:

- $F_{cap} = 2\pi R\gamma_c\left[1 - \frac{1}{\sqrt{1+\frac{2V_B}{2RD^2}}}\right]$

- $V(t) = V_m\left[1 - exp\left(-\frac{C_0 h_{ij}^3}{V_m \eta} t\right)\right]$

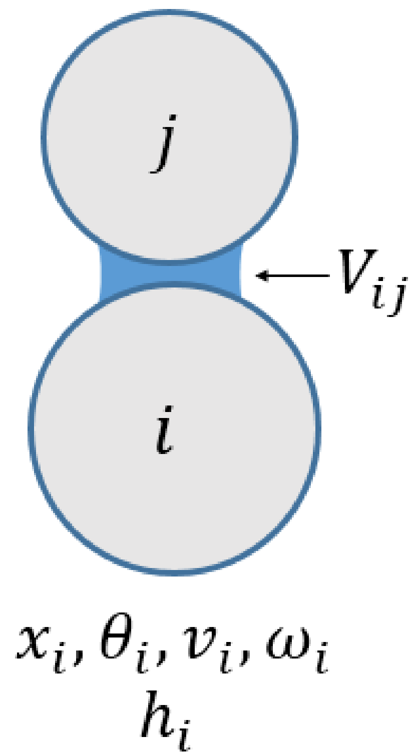
- $S_c = R(1 + \frac{\theta}{2})V^{1/3}$

- $F_{vis} = -\frac{3}{2}\pi\eta R^2 \frac{1}{D}\frac{dD}{dt}$

- $F_{Bridge} = F_{cap} + F_{vis}$

- Particle Hookean contact with friction and rotation.

- Conserving the volume of the water in the system



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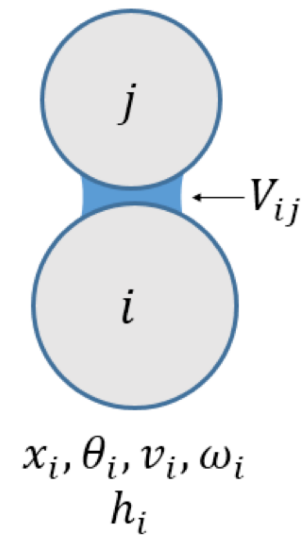
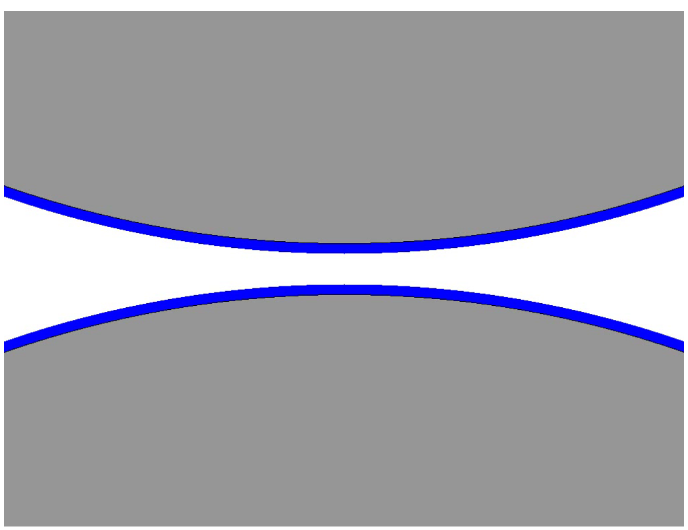
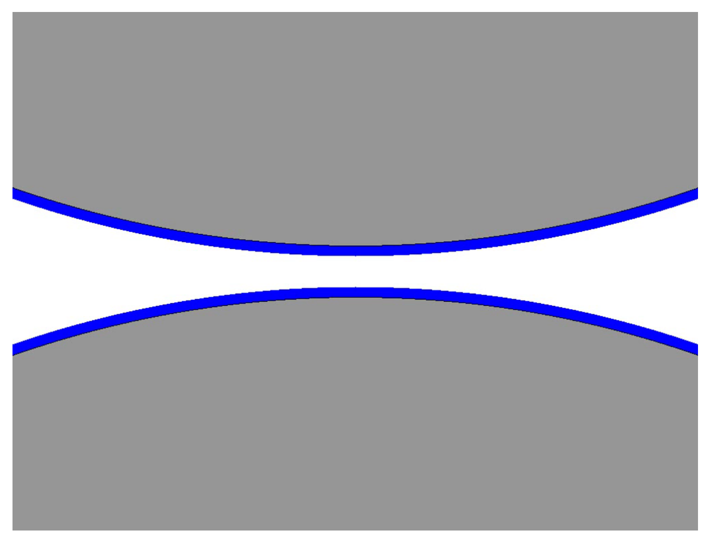
Fluid-extended DEM interaction:



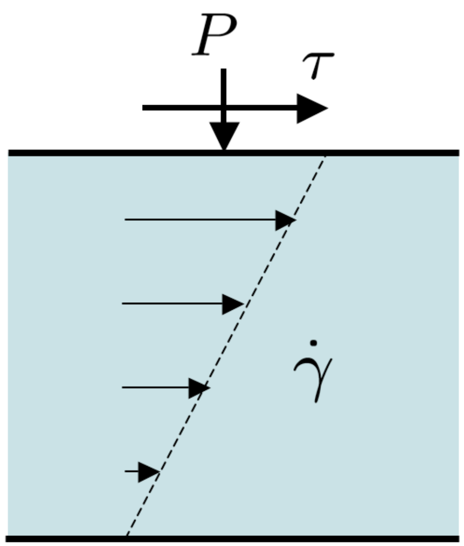
Fast collision of wet grains



Slow collision of wet grains

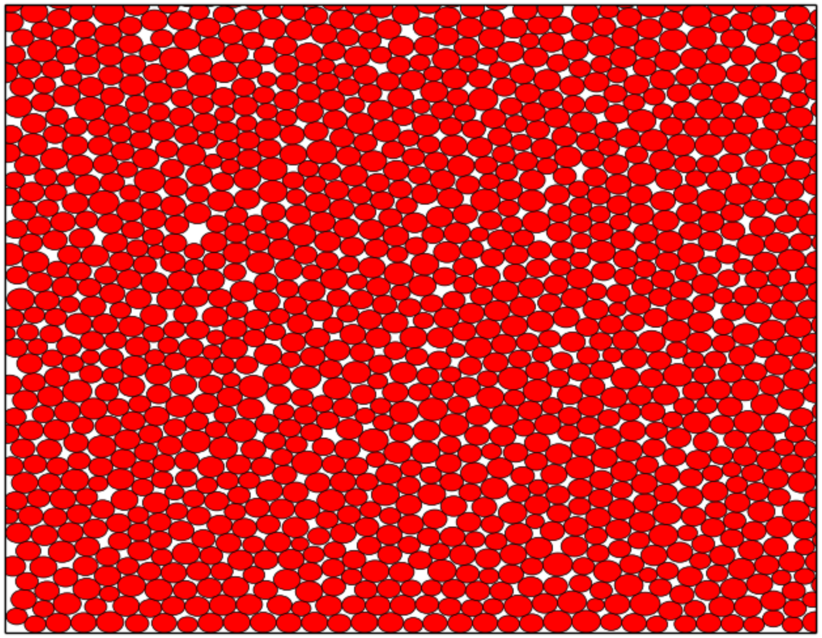


Hunting for a homogenized wet grain rheology:

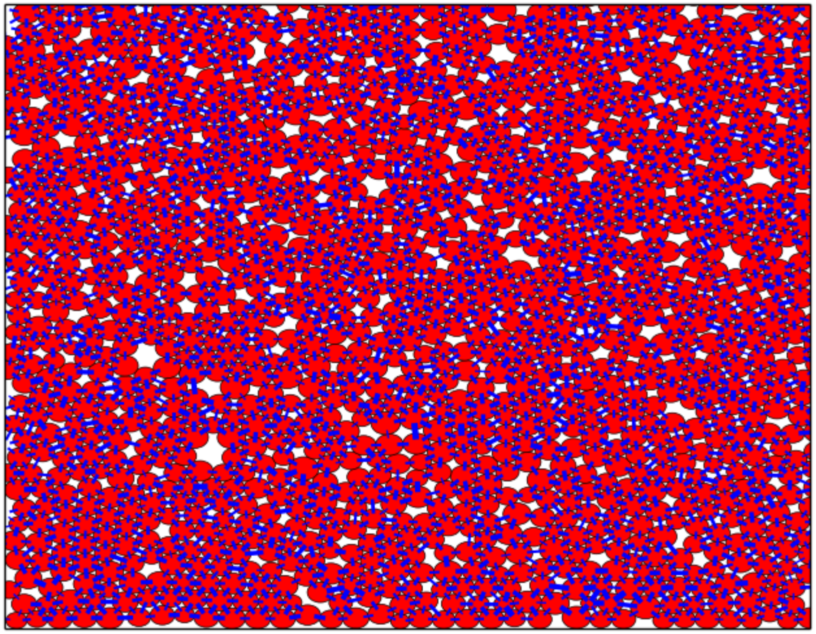


$\mu = \tau / P$

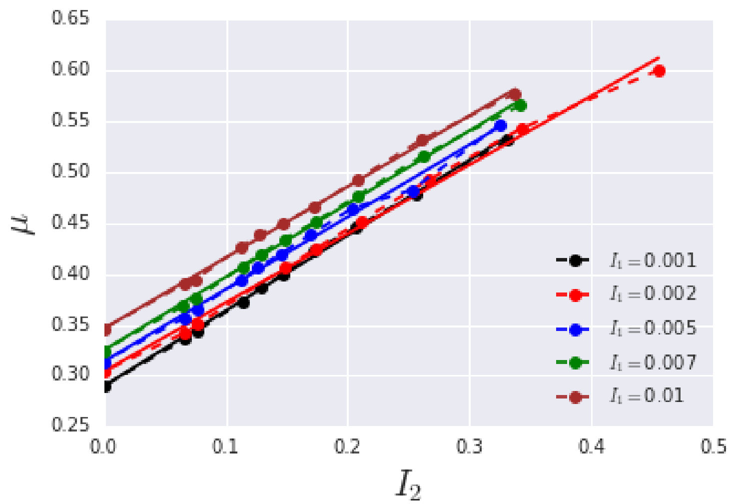
Dry

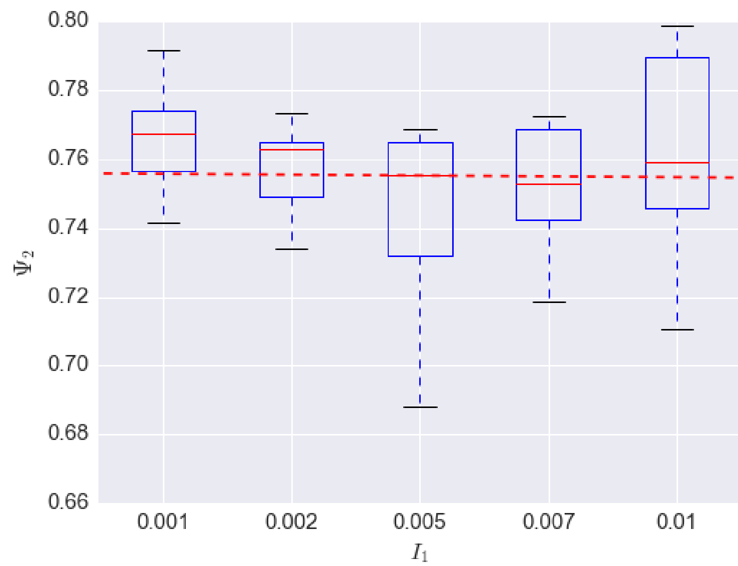


Wet



Results





$$I_1 = \dot{\epsilon}_{xy}\sqrt{\frac{m}{P}}, I_2 = \frac{\gamma_c}{Pd}$$

$$\tau = P\hat{\Psi}_1(I_1) + PI_2\hat{\Psi}_2(I_1) \Rightarrow \Psi_2(I_1) = \frac{<d>(\tau - P\Psi_1(I_1))}{\gamma_c}$$

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